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Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.009\text{ \AA}$
 R factor = 0.042
 wR factor = 0.117
Data-to-parameter ratio = 15.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**catena-Poly[[silver(I)- μ -1,4-diamino-
butane- $\kappa^2\text{N:N}'$] hexafluoroarsenate]**The title compound, $\{[\text{Ag}(\text{C}_4\text{H}_{12}\text{N}_2)](\text{AsF}_6)\}_n$, is a helical one-dimensional chain Ag^{I} complex. The Ag^{I} atom is coordinated by two N atoms from two 1,4-diaminobutane ligands, in a nearly linear geometry. The crystal structure is a three-dimensional structure stabilized by $\text{N}-\text{H}\cdots\text{F}$ hydrogen bonds and weak $\text{Ag}\cdots\text{F}$ interactions.Received 29 August 2003
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Comment

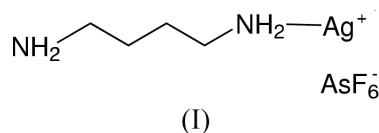
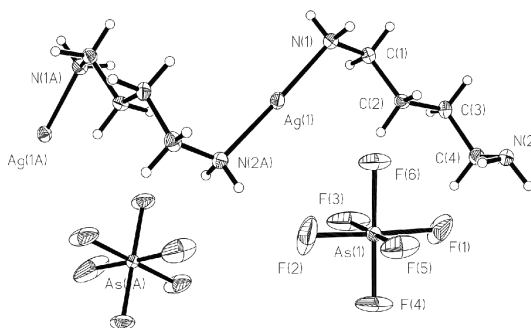
The title complex, (I), crystallizes in the monoclinic space group $P2_1/n$. The complex consists of polymeric 1,4-diaminobutanesilver(I) cations and hexafluoroarsenate counterions as shown in Fig. 1. The simplest repeat unit is the 1,4-diaminobutanesilver(I) cation and a hexafluoroarsenate anion. In the cation, the Ag atom is in a linear coordination environment, being coordinated by two N atoms from different butanediamine ligands. The average $\text{Ag}-\text{N}$ distance is $2.137(5)\text{ \AA}$ and the angle around Ag^{I} is $178.1(2)^\circ$, indicating a slightly distorted linear geometry at the Ag^{I} atom.All the butane ligands are fully extended in different directions and are linked together by the $\text{Ag}-\text{N}$ bonds, forming a one-dimensional chain along the c axis (see Fig. 2).In the crystal structure, extensive intermolecular hydrogen bonds ($\text{N}2-\text{H}2\text{C}\cdots\text{F}1$, $\text{N}1-\text{H}1\text{C}\cdots\text{F}1^{\text{i}}$ and $\text{N}2-\text{H}2\text{D}\cdots\text{F}2^{\text{ii}}$; for symmetry codes see Table 1), and weak interactions between the Ag atom and the F atoms [$\text{Ag}1\cdots\text{F}3 = 3.462(7)\text{ \AA}$, $\text{Ag}1\cdots\text{F}4^{\text{iii}} = 3.353(7)\text{ \AA}$, $\text{Ag}1\cdots\text{F}5^{\text{iv}} =$ 

Figure 1

The structure of the title compound, showing 20% probability displacement ellipsoids and the atom-numbering scheme.

3.241 (7) Å, $\text{Ag1}\cdots\text{F6} = 3.208 (7) \text{ \AA}$ and $\text{Ag1}\cdots\text{F6}^{\text{iv}} = 3.126 (7) \text{ \AA}$] were observed [symmetry codes: (iii) $x - \frac{1}{2}$, $-y + \frac{3}{2}$, $z + \frac{1}{2}$; (iv) $-x$, $-y + 2$, $-z + 1$].

Experimental

All reagents and solvents were used as obtained without further purification. AgAsF_6 (0.5 mmol, 148 mg) and 1,4-diaminobutane (0.5 mmol, 44 mg) were dissolved in ammonia (10 ml). The mixture was stirred for *ca* 10 min to give a clear solution. After allowing the solution to stand in air for 3 d with gradual loss of ammonia gas, large colorless crystals were formed. The crystals were filtered off and washed three times with water and dried in a vacuum desiccator using anhydrous CaCl_2 (yield 63%). Elemental analysis found: C 12.59, H 3.21, N 7.18%; calculated for $\text{C}_4\text{H}_{12}\text{AgAsF}_6\text{N}_2$: C 12.48, H 3.14, N 7.28%.

Crystal data

$[\text{Ag}(\text{C}_4\text{H}_{12}\text{N}_2)](\text{AsF}_6)$
 $M_r = 384.95$
 Monoclinic, $P2_1/n$
 $a = 7.806 (2) \text{ \AA}$
 $b = 10.371 (2) \text{ \AA}$
 $c = 13.234 (3) \text{ \AA}$
 $\beta = 105.74 (3)^\circ$
 $V = 1031.2 (4) \text{ \AA}^3$
 $Z = 4$

$D_x = 2.480 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 4450 reflections
 $\theta = 2.8\text{--}25.4^\circ$
 $\mu = 5.19 \text{ mm}^{-1}$
 $T = 293 (2) \text{ K}$
 Block, colorless
 $0.38 \times 0.32 \times 0.20 \text{ mm}$

Data collection

Siemens SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.155$, $T_{\text{max}} = 0.366$
 4479 measured reflections

2025 independent reflections
 1757 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$
 $\theta_{\text{max}} = 26.0^\circ$
 $h = -9 \rightarrow 9$
 $k = -12 \rightarrow 8$
 $l = -14 \rightarrow 16$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.117$
 $S = 1.08$
 2025 reflections
 135 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0714P)^2 + 0.904P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 1.22 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.90 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bonding geometry (Å, °).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
$\text{N2--H2C}\cdots\text{F1}$	0.91 (8)	2.17 (8)	2.987 (8)	150 (7)
$\text{N1--H1C}\cdots\text{F1}^{\text{i}}$	0.90	2.11	3.012 (7)	175
$\text{N2--H2D}\cdots\text{F2}^{\text{ii}}$	0.81 (7)	2.23 (7)	3.018 (8)	165 (6)

Symmetry codes: (i) $x - \frac{1}{2}$, $\frac{3}{2} - y$, $\frac{1}{2} + z$; (ii) $x - \frac{1}{2}$, $\frac{3}{2} - y$, $z - \frac{1}{2}$.

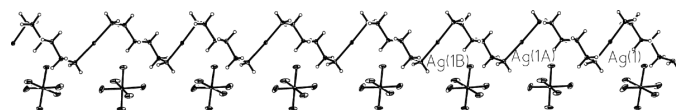


Figure 2

The one-dimensional helical chain of (I), viewed along c .

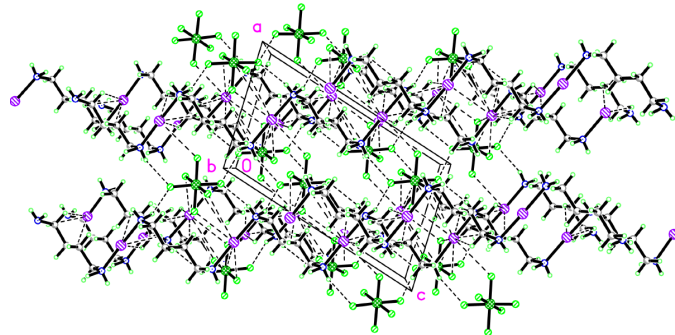


Figure 3

The crystal packing of (I), showing the hydrogen-bonding interactions as dashed lines.

H atoms H2C and H2D were located in Fourier maps and were refined isotropically. All the other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with N—H and C—H distances of 0.90 and 0.96 Å, respectively; the U_{eq} values for these H atoms were fixed at 0.08 \AA^2 . The F atoms have quite large U_{eq} values, but they were not considered disordered. The highest peak is located at (0.2765, 0.2301, 0.0467).

Data collection: SMART (Siemens, 1996); cell refinement: SMART; data reduction: SAINT (Siemens, 1996); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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